

10670105 HydroformylationEthyUnsatCmp 407578-79-4

=> s 407578-79-4/rn
L7 1 407578-79-4/RN

=> fil hcap

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.45

72.51

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FILE COVERS 1907 - 19 Feb 2007 VOL 146 ISS 9

FILE LAST UPDATED: 18 Feb 2007 (20070218/ED)

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=> s 17
L8 3 L7

=> d ibib abs 18 1-3

L8 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:141010 HCAPLUS

DOCUMENT NUMBER: 142:221614

TITLE: Carbonylation of conjugated dienes using palladium-phosphine complex catalysts with improved stability

INVENTOR(S): Sielcken, Otto Erik; Baur, Henricus Anna Christiaan; Toth, Imre

PATENT ASSIGNEE(S): DSM IP Assets B. V., Neth.

SOURCE: PCT Int. Appl., 37 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|--|------|----------|-----------------|----------|
| WO 2005014520 | A1 | 20050217 | WO 2004-EP7059 | 20040628 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, | | | | |

GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
 RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

EP 1656336 A1 20060517 EP 2004-740443 20040628
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK

CN 1829679 A 20060906 CN 2004-80021621 20040628
 PRIORITY APPLN. INFO.: EP 2003-77340 A 20030725 X
 WO 2004-EP7059 W 20040628

OTHER SOURCE(S): CASREACT 142:221614; MARPAT 142:221614

AB A process for carbonylation of a conjugated diene is carried out by reacting the conjugated diene with carbon monoxide and a hydroxyl group-containing compound in the presence of a palladium catalyst system in a reaction zone to produce a reaction mixture, the catalyst system comprising (a) a source of palladium cations, (b) a mono-, bi- or multidentate phosphine ligand, containing at least one phosphorus atom directly bound to two or three aliphatic carbon atoms, as a process ligand to produce a palladium-phosphine ligand complex catalyst, and (c) a source of anions selected from carboxylic acid and halide ions. The process ligand (b) contains a moiety of the formula $X-P(A1)(A2)$, where A1 and A2 each represent an aliphatic carbon atom which may be connected to one or more aliphatic or aromatic carbon atoms or both A1 and A2 may be a part of at least 5-membered ring including the phosphorus atom, and X represents an aliphatic or aromatic carbon atom which may be connected to one or more aliphatic or aromatic

carbon atoms or X is a part of an organic bridging group connecting another identically or differently substituted phosphorus atom, the process ligand being fed continuously or periodically to the process as a ligand make-up at a temperature $\leq 50^\circ$. The catalysts have improved stability to degradation during the reaction and can be efficiently regenerated and in-process recycled. Thus, a homogeneous catalyst was prepared by dissolving under nitrogen palladium acetate (370 mg), 2,3-bis(9-phosphabicyclononyl)butane (589 mg) and pivalic acid (1.96 g) in freshly distilled Me pentenoates (98.9 g), and adding 21.6 μ L of a 57%-aqueous hydrogen iodide. The catalyst showed selectivity of 87% after 86 h of use in a continuous carbonylation of butadiene into Me pentenoates carried out at 135° with parallel feeding of carbon monoxide, butadiene, the catalyst solution, and methanol, addnl. methanol solns. of 2,3-bis(9-phosphabicyclononyl)butane (166 mg/L) and pivalic acid (35 g/L) being fed into the catalyst feed line at room temperature

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:287803 HCAPLUS

DOCUMENT NUMBER: 140:310272

TITLE: Process for the hydroformylation of an ethylenically unsaturated compound

INVENTOR(S): Drent, Eit; Van Ginkel, Roelof; Jager, Willem Wabe

PATENT ASSIGNEE(S): Shell Internationale Research Maatschappij B.V., Neth.

SOURCE: PCT Int. Appl., 28 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|--|------|----------|-----------------|------------|
| WO 2004028689 | A2 | 20040408 | WO 2003-EP50654 | 20030924 |
| WO 2004028689 | A3 | 20040729 | | |
| W: | | | | |
| AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| RW: | | | | |
| GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| CA 2500095 | A1 | 20040408 | CA 2003-2500095 | 20030924 |
| AU 2003299066 | A1 | 20040419 | AU 2003-299066 | 20030924 |
| US 2004167362 | A1 | 20040826 | US 2003-670105 | 20030924 |
| EP 1542798 | A2 | 20050622 | EP 2003-798198 | 20030924 |
| R: | | | | |
| AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK | | | | |
| CN 1684769 | A | 20051019 | CN 2003-823006 | 20030924 |
| JP 2006500415 | T | 20060105 | JP 2004-539074 | 20030924 |
| ZA 2005002080 | A | 20050912 | ZA 2005-2080 | 20050311 |
| PRIORITY APPLN. INFO.: | | | EP 2002-256696 | A 20020926 |
| | | | WO 2003-EP50654 | W 20030924 |

OTHER SOURCE(S): MARPAT 140:310272

AB The present invention relates to a process for the hydroformylation of an optionally substituted ethylenically unsatd. compound by reaction thereof with carbon monoxide and hydrogen in the presence of a specific catalyst system. The specific catalyst system comprises (A) a source of group VIII metal cations, (B) a diphosphine ligand having the general formula X_1RX_2 , (C) an acid with $pK_a < 3$, measured in an aqueous solution at 18° or a salt derived thereof, and (D) a source of halide anions, wherein X_1 , X_2 = independently an optionally substituted cyclic group with ≥ 5 ring atoms, of which one is a phosphorus atom, and R = a bivalent optionally substituted bridging group, connected to each phosphorus atom by a sp^2 hybridized carbon atom. Furthermore some specific bidentate diphosphines used in this process are described. Thus, 1,2-dibromobenzene 9.44, 1,4-diazabicyclo[2,2,2]octane 22.4, 9-phosphabicyclo[3.3.1]nonane 13.0, and tetrakis(triphenylphosphine)palladium 2.32 g were heated at 140° to give 7.10 g (yield 50%) 1,2-bis(9-phosphabicyclo[3.3.1]nonyl)benzene, 0.40 mmol of which was mixed with methane sulfonic acid 1.0, hydrochloric acid 0.20, and palladium acetate 0.25 mmol, and 20 mL 1-octene and heated at 120° for 5 h under 20 bar carbon monoxide and 40 bar hydrogen to give an alkanol product >99, a linear alkanol product 68, and a hydrogenation product <1%.

L8 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:256216 HCAPLUS

DOCUMENT NUMBER: 136:296537

TITLE: Process and palladium-diphosphine catalyst system for the carbonylation of conjugated dienes

INVENTOR(S): Drent, Eit; Jager, Willem Wabe; Sielcken, Otto Erik; Toth, Imre

PATENT ASSIGNEE(S): DSM N.V., Neth.

SOURCE: PCT Int. Appl., 28 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|--------------------|------------|
| WO 2002026690 | A1 | 20020404 | WO 2001-NL709 | 20010926 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| AU 2002011067 | A5 | 20020408 | AU 2002-11067 | 20010926 |
| EP 1332124 | A1 | 20030806 | EP 2001-979078 | 20010926 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR | | | | |
| US 2004039226 | A1 | 20040226 | US 2003-381040 | 20030825 |
| US 6835850 | B2 | 20041228 | | |
| PRIORITY APPLN. INFO.: | | | EP 2000-203355 | A 20000927 |
| | | | EP 2000-203356 | A 20000927 |
| | | | EP 2000-2000203355 | A 20000927 |
| | | | EP 2000-2000203356 | A 20000927 |
| | | | WO 2001-NL709 | W 20010926 |

OTHER SOURCE(S): MARPAT 136:296537

AB Conjugated dienes (e.g., 1,3-butadiene) are readily subjected to carbonylation to produce unsatd. esters (e.g., Me 3-pentenoate which is an adipate ester precursor) by reacting the conjugated diene with carbon monoxide and an hydroxyl group-containing compound (e.g., methanol) in the presence of a catalyst system based on: (a) a source of palladium cations (e.g., palladium acetate); (b) a diphosphine ligand X1RX2 (X1, X2 = cyclic group with at least 5 ring atoms of which one is a phosphorus atom; R = bivalent aliphatic bridging group, connecting both phosphorus atoms containing from 2 to 4 atoms in the bridge which is substituted with at least one substituent, Ph group with both phosphorus groups bound to the 1,2-position); and (c) a source of anions (e.g., pivalic acid).

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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(FILE 'HOME' ENTERED AT 14:28:12 ON 19 FEB 2007)

FILE 'HCAPLUS' ENTERED AT 14:28:22 ON 19 FEB 2007
 E US20040167362/PN,PRN,AN

L1 1 S E3

FILE 'REGISTRY' ENTERED AT 14:29:00 ON 19 FEB 2007
 L2 0 S L1

FILE 'HCAPLUS' ENTERED AT 14:29:41 ON 19 FEB 2007
 E US20040167362/PN,PRN,AN

10670105 HydroformylationEthyUnsatCmp 407578-79-4

L3 1 S E3

FILE 'REGISTRY' ENTERED AT 14:31:23 ON 19 FEB 2007

L4 0 S E1-E12

L5 1 S 676992-18-0/RN

FILE 'HCAPLUS' ENTERED AT 14:33:07 ON 19 FEB 2007

L6 1 S L5

FILE 'REGISTRY' ENTERED AT 14:34:18 ON 19 FEB 2007

L7 1 S 407578-79-4/RN

FILE 'HCAPLUS' ENTERED AT 14:34:29 ON 19 FEB 2007

L8 3 S L7

10670105 HydroformylationEthyUnsatCmp

676992-15-7

=> s 676992-15-7/rn
L9 1 676992-15-7/RN

=> file hcap

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.45

99.65

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

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-2.34

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FILE LAST UPDATED: 18 Feb 2007 (20070218/ED)

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=> s l9
L10 2 L9

=> d ibib abs l10 1-2

L10 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:473316 HCAPLUS

DOCUMENT NUMBER: 145:145808

TITLE: Highly Selective Halide Anion-Promoted
Palladium-Catalyzed Hydroformylation of Internal
Alkenes to Linear Alcohols

AUTHOR(S): Konya, Denes; Lenero, Karina Q. Almeida; Drent, Eite

CORPORATE SOURCE: Shell Global Solutions, Amsterdam, 1030BN, Neth.

SOURCE: Organometallics (2006), 25(13), 3166-3174

CODEN: ORGND7; ISSN: 0276-7333

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 145:145808

AB The authors report on their study of the Pd-catalyzed hydroformylation of alkenes. A (bcope)Pd(OTf)₂ complex [bcope = 1,2-bis[(cyclooctyl)phosphino]ethane] with sub-stoichiometrically added halide

anions is a highly efficient homogeneous catalyst (precursor) to selectively convert internal linear alkenes into predominantly linear (detergent) alcs. under mild conditions. Halide anion-dependent effects on the hydroformylation reaction rate as well as its chemo- and regioselectivity are observed. Thus, the rate of hydroformylation of thermally equilibrated internal higher alkenes increases by a factor of .apprx.6-7 with chloride/bromide and about a factor 3-4 with iodide, while the selectivity toward alcs. increases to almost 100% upon addition of a substoichiometric quantity (with respect to Pd) of the halide anion source. Curiously, the regioselectivity toward linear alc. increases in the reverse order, i.e., iodide > bromide > chloride. From a detailed anal. of the products obtained with model substrates, hydrogenolysis of (bcope)palladium-acyl intermediates is strongly accelerated by the presence of halide anions. From a comparison of the catalytic performance with some related L2Pd(OTf)2 complexes, in which L2 are bidentate phosphines closely related to bcope, it also appears that the ligand plays a critical role in the promoting effect of halide anions.

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:287803 HCAPLUS

DOCUMENT NUMBER: 140:310272

TITLE: Process for the hydroformylation of an ethylenically unsaturated compound

INVENTOR(S): Drent, Eit; Van Ginkel, Roelof; Jager, Willem Wabe

PATENT ASSIGNEE(S): Shell Internationale Research Maatschappij B.V., Neth.

SOURCE: PCT Int. Appl., 28 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|--|----------|-----------------|------------|
| WO 2004028689 | A2 | 20040408 | WO 2003-EP50654 | 20030924 |
| WO 2004028689 | A3 | 20040729 | | |
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| CA 2500095 | A1 | 20040408 | CA 2003-2500095 | 20030924 |
| AU 2003299066 | A1 | 20040419 | AU 2003-299066 | 20030924 |
| US 2004167362 | A1 | 20040826 | US 2003-670105 | 20030924 |
| EP 1542798 | A2 | 20050622 | EP 2003-798198 | 20030924 |
| R: | AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK | | | |
| CN 1684769 | A | 20051019 | CN 2003-823006 | 20030924 |
| JP 2006500415 | T | 20060105 | JP 2004-539074 | 20030924 |
| ZA 2005002080 | A | 20050912 | ZA 2005-2080 | 20050311 |
| PRIORITY APPLN. INFO.: | | | EP 2002-256696 | A 20020926 |
| | | | WO 2003-EP50654 | W 20030924 |

*Int
app*

OTHER SOURCE(S): MARPAT 140:310272

AB The present invention relates to a process for the hydroformylation of an optionally substituted ethylenically unsatd. compound by reaction thereof with carbon monoxide and hydrogen in the presence of a specific catalyst system. The specific catalyst system comprises (A) a source of group VIII metal cations, (B) a diphosphine ligand having the general formula X_1RX_2 , (C) an acid with $pK_a < 3$, measured in an aqueous solution at 18° or a salt derived thereof, and (D) a source of halide anions, wherein X_1 , X_2 = independently an optionally substituted cyclic group with ≥ 5 ring atoms, of which one is a phosphorus atom, and R = a bivalent optionally substituted bridging group, connected to each phosphorus atom by a sp^2 hybridized carbon atom. Furthermore some specific bidentate diphosphines used in this process are described. Thus, 1,2-dibromobenzene 9.44, 1,4-diazabicyclo[2,2,2]octane 22.4, 9-phosphabicyclo[3.3.1]nonane 13.0, and tetrakis(triphenylphosphine)palladium 2.32 g were heated at 140° to give 7.10 g (yield 50%) 1,2-bis(9-phosphabicyclo[3.3.1]nonyl)benzene, 0.40 mmol of which was mixed with methane sulfonic acid 1.0, hydrochloric acid 0.20, and palladium acetate 0.25 mmol, and 20 mL 1-octene and heated at 120° for 5 h under 20 bar carbon monoxide and 40 bar hydrogen to give an alkanol product >99, a linear alkanol product 68, and a hydrogenation product <1%.

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E US20040167362/PN,PRN,AN

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FILE 'REGISTRY' ENTERED AT 14:29:00 ON 19 FEB 2007

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FILE 'HCAPLUS' ENTERED AT 14:29:41 ON 19 FEB 2007

E US20040167362/PN,PRN,AN

L3 1 S E3

FILE 'REGISTRY' ENTERED AT 14:31:23 ON 19 FEB 2007

L4 0 S E1-E12

L5 1 S 676992-18-0/RN

FILE 'HCAPLUS' ENTERED AT 14:33:07 ON 19 FEB 2007

L6 1 S L5

FILE 'REGISTRY' ENTERED AT 14:34:18 ON 19 FEB 2007

L7 1 S 407578-79-4/RN

FILE 'HCAPLUS' ENTERED AT 14:34:29 ON 19 FEB 2007

L8 3 S L7

FILE 'REGISTRY' ENTERED AT 14:38:30 ON 19 FEB 2007

L9 1 S 676992-15-7/RN

FILE 'HCAPLUS' ENTERED AT 14:38:42 ON 19 FEB 2007

L10 2 S L9

=> s 676992-16-8/rn
L11 1 676992-16-8/RN

=> fil hcap

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.45

116.16

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

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-3.90

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FILE LAST UPDATED: 18 Feb 2007 (20070218/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l11
L12 1 L11

=> d scan

L12 1 ANSWERS HCAPLUS COPYRIGHT 2007 ACS on STN

IC ICM B01J031-24

ICS B01J027-08; B01J031-02; C07F009-6568; C07F015-00; C07C045-50

CC 67-1 (Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms)
Section cross-reference(s): 23

TI Process for the hydroformylation of an ethylenically unsaturated compound
ST process hydroformylation ethylenically unsatd compd;
bisphosphabicyclononylbenzene ligand palladium acetate catalyst octene
hydroformylation

IT Alkenes, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(C11-12; hydroformylation of ethylenically unsatd. compds.)

IT Ligands

RL: CAT (Catalyst use); USES (Uses)

(bidentate, diphosphines, hydroformylation catalyst ligand;
hydroformylation of ethylenically unsatd. compds.)

IT Hydroformylation

(hydroformylation of ethylenically unsatd. compds.)
 IT Group VIII elements
 RL: CAT (Catalyst use); USES (Uses)
 (hydroformylation of ethylenically unsatd. compds.)
 IT Catalysts
 (hydroformylation; hydroformylation of ethylenically unsatd. compds.)
 IT 676992-18-0 676992-19-1
 RL: CAT (Catalyst use); USES (Uses)
 (hydroformylation catalyst ligand; hydroformylation of ethylenically unsatd. compds.)
 IT 407578-79-4P, 9-Phosphabicyclo[3.3.1]nonane, 9,9'-(1,2-phenylene)bis-
 676992-15-7P 676992-16-8P
 RL: CAT (Catalyst use); IMF (Industrial manufacture); PREP (Preparation);
 USES (Uses)
 (hydroformylation catalyst ligand; hydroformylation of ethylenically unsatd. compds.)
 IT 3375-31-3
 RL: CAT (Catalyst use); USES (Uses)
 (hydroformylation of ethylenically unsatd. compds.)
 IT 4547-43-7P, Hexanoic acid, 6-hydroxy-, methyl ester 167707-57-5P,
 Pentanoic acid, 5-hydroxy-4-methyl-, methyl ester 676992-17-9P
 RL: IMF (Industrial manufacture); PREP (Preparation)
 (hydroformylation of ethylenically unsatd. compds.)
 IT 111-66-0, 1-Octene 630-08-0, Carbon monoxide, reactions 818-59-7
 1333-74-0, Hydrogen, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (hydroformylation of ethylenically unsatd. compds.)
 IT 583-53-9, 1,2-Dibromobenzene 3141-26-2, 3,4-Dibromothiophene
 13887-02-0, 9-Phosphabicyclo[3.3.1]nonane 75415-78-0,
 1,2-Dibromocyclopentene
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reactant in hydroformylation catalyst ligand preparation; hydroformylation of ethylenically unsatd. compds.)

ALL ANSWERS HAVE BEEN SCANNED

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FILE 'HCAPLUS' ENTERED AT 14:28:22 ON 19 FEB 2007

E US20040167362/PN,PRN,AN

L1 1 S E3

FILE 'REGISTRY' ENTERED AT 14:29:00 ON 19 FEB 2007

L2 0 S L1

FILE 'HCAPLUS' ENTERED AT 14:29:41 ON 19 FEB 2007

E US20040167362/PN,PRN,AN

L3 1 S E3

FILE 'REGISTRY' ENTERED AT 14:31:23 ON 19 FEB 2007

L4 0 S E1-E12

L5 1 S 676992-18-0/RN

FILE 'HCAPLUS' ENTERED AT 14:33:07 ON 19 FEB 2007

L6 1 S L5

10670105 HydroformylationEthyUnsatCmp 676992-16-8

L7 FILE 'REGISTRY' ENTERED AT 14:34:18 ON 19 FEB 2007
1 S 407578-79-4/RN

L8 FILE 'HCAPLUS' ENTERED AT 14:34:29 ON 19 FEB 2007
3 S L7

L9 FILE 'REGISTRY' ENTERED AT 14:38:30 ON 19 FEB 2007
1 S 676992-15-7/RN

L10 FILE 'HCAPLUS' ENTERED AT 14:38:42 ON 19 FEB 2007
2 S L9

L11 FILE 'REGISTRY' ENTERED AT 14:41:02 ON 19 FEB 2007
1 S 676992-16-8/RN

L12 FILE 'HCAPLUS' ENTERED AT 14:41:16 ON 19 FEB 2007
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10670105 HydroformylationEthyUnsatCmp 676992-19-1

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L13 1 676992-19-1/RN

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| => fil hcap | | |
| COST IN U.S. DOLLARS | SINCE FILE | TOTAL |
| | ENTRY | SESSION |
| FULL ESTIMATED COST | 0.45 | 124.41 |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE | TOTAL |
| | ENTRY | SESSION |
| CA SUBSCRIBER PRICE | 0.00 | -3.90 |

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L14 1 L13

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L14 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:287803 HCAPLUS
DOCUMENT NUMBER: 140:310272
TITLE: Process for the hydroformylation of an ethylenically unsaturated compound *Drent APP*
INVENTOR(S): Drent, Eit; Van Ginkel, Roelof; Jager, Willem Wabe
PATENT ASSIGNEE(S): Shell Internationale Research Maatschappij B.V., Neth.
SOURCE: PCT Int. Appl., 28 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---------------|------|----------|-----------------|----------|
| WO 2004028689 | A2 | 20040408 | WO 2003-EP50654 | 20030924 |

WO 2004028689 A3 20040729

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

CA 2500095 A1 20040408 CA 2003-2500095 20030924

AU 2003299066 A1 20040419 AU 2003-299066 20030924

US 2004167362 A1 20040826 US 2003-670105 20030924

EP 1542798 A2 20050622 EP 2003-798198 20030924

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK

CN 1684769 A 20051019 CN 2003-823006 20030924

JP 2006500415 T 20060105 JP 2004-539074 20030924

ZA 2005002080 A 20050912 ZA 2005-2080 20050311

PRIORITY APPLN. INFO.: EP 2002-256696 A 20020926

WO 2003-EP50654 W 20030924

OTHER SOURCE(S): MARPAT 140:310272

AB The present invention relates to a process for the hydroformylation of an optionally substituted ethylenically unsatd. compound by reaction thereof with carbon monoxide and hydrogen in the presence of a specific catalyst system. The specific catalyst system comprises (A) a source of group VIII metal cations, (B) a diphosphine ligand having the general formula X_1RX_2 , (C) an acid with $pK_a < 3$, measured in an aqueous solution at 18° or a salt derived thereof, and (D) a source of halide anions, wherein X_1 , X_2 = independently an optionally substituted cyclic group with ≥ 5 ring atoms, of which one is a phosphorus atom, and R = a bivalent optionally substituted bridging group, connected to each phosphorus atom by a sp^2 hybridized carbon atom. Furthermore some specific bidentate diphosphines used in this process are described. Thus, 1,2-dibromobenzene 9.44, 1,4-diazabicyclo[2,2,2]octane 22.4, 9-phosphabicyclo[3.3.1]nonane 13.0, and tetrakis(triphenylphosphine)palladium 2.32 g were heated at 140° to give 7.10 g (yield 50%) 1,2-bis(9-phosphabicyclo[3.3.1]nonyl)benzene, 0.40 mmol of which was mixed with methane sulfonic acid 1.0, hydrochloric acid 0.20, and palladium acetate 0.25 mmol, and 20 mL 1-octene and heated at 120° for 5 h under 20 bar carbon monoxide and 40 bar hydrogen to give an alkanol product >99, a linear alkanol product 68, and a hydrogenation product <1%.

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L1 1 S E3

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L2 0 S L1

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L3 E US20040167362/PN,PRN,AN
1 S E3

L4 FILE 'REGISTRY' ENTERED AT 14:31:23 ON 19 FEB 2007
0 S E1-E12
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L7 FILE 'REGISTRY' ENTERED AT 14:34:18 ON 19 FEB 2007
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L11 FILE 'REGISTRY' ENTERED AT 14:41:02 ON 19 FEB 2007
1 S 676992-16-8/RN

L12 FILE 'HCAPLUS' ENTERED AT 14:41:16 ON 19 FEB 2007
1 S L11

L13 FILE 'REGISTRY' ENTERED AT 14:42:48 ON 19 FEB 2007
1 S 676992-19-1/RN

L14 FILE 'HCAPLUS' ENTERED AT 14:43:03 ON 19 FEB 2007
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10670105 HydroformylationEthyUnsatCmp claim 11

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L13 1 S 676992-19-1/RN

FILE 'HCAPLUS' ENTERED AT 14:43:03 ON 19 FEB 2007

L14 1 S L13

FILE 'HCAPLUS' ENTERED AT 14:44:18 ON 19 FEB 2007

S "1,2-P,P'BIS(9-PHOSPHABICYCLONONYL) BENZENE"/CN

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L15 0 S "1,2-P,P'BIS(9-PHOSPHABICYCLONONYL) BENZENE"/CN

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L16 0 S L15

S "BENZENE 1,2-P,P'BIS(9-PHOSPHABICYCLONONYL)/CN

FILE 'REGISTRY' ENTERED AT 14:45:32 ON 19 FEB 2007

L17 0 S "BENZENE 1,2-P,P'BIS(9-PHOSPHABICYCLONONYL)/CN

10670105 HydroformylationEthyUnsatCmp claim 11

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L22 0 S "THIOPHENE, 3,4-P,P'BIS(9-PHOSPHABICYCLONONYL"
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L23 0 S "THIOPHENE, 3,4-P,P'BIS(9-PHOSPHABICYCLONONYL)/CN

FILE 'HCAPLUS' ENTERED AT 14:47:41 ON 19 FEB 2007
L24 0 S L23